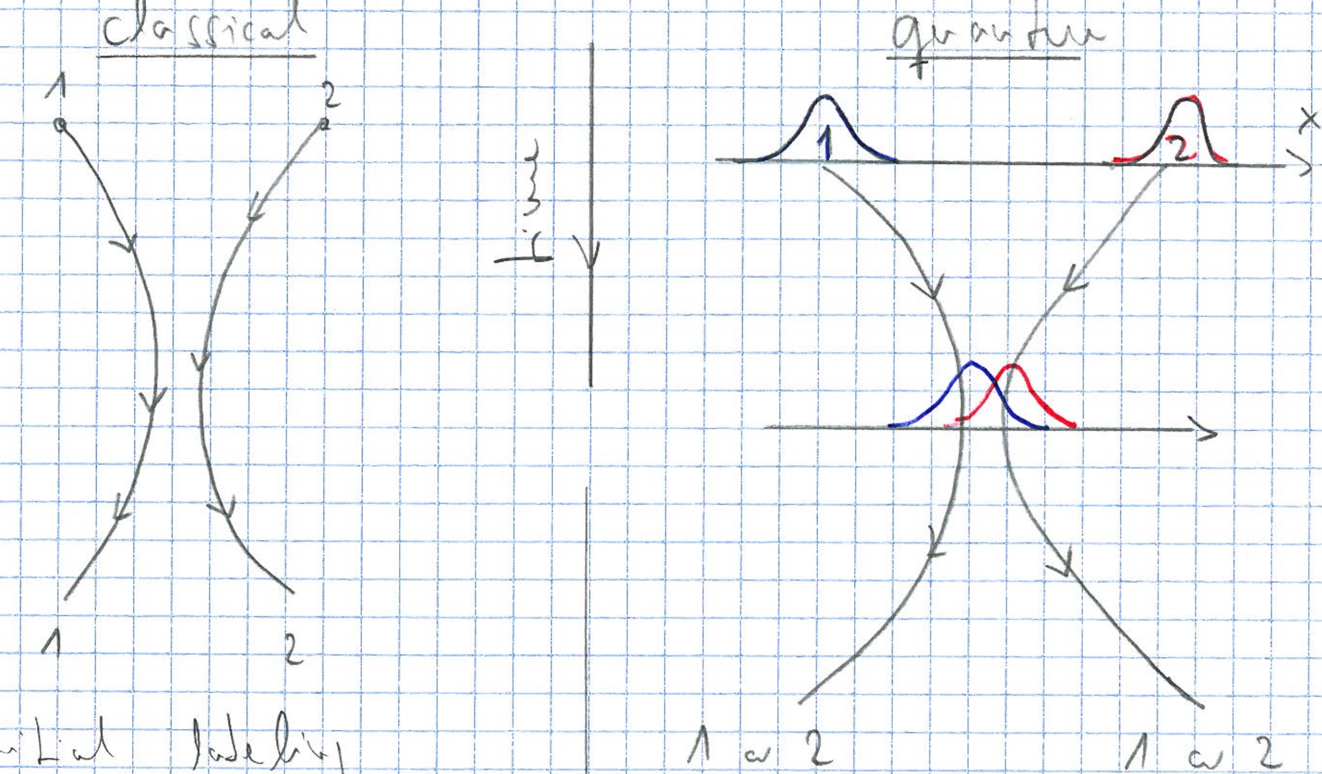
II. Second quantization

1° Indistinguishability

Identical quantum particles are fundamentally indistinguishable :



- initial labeling persists because each particle has a distinct trajectory at all times

- identity of particles is lost when their wave packets overlap

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As a consequence of indistinguishability, a additional symmetry postulate has to be introduced for systems of identical particles.

c) Permutation operators

Consider a N-particle wave function

$$\psi(x_1,\dots,x_N) = \langle x_1|\langle x_2\dots\langle x_N|\psi\rangle$$

$$\begin{cases} x_i = (\vec{r}_i, s_i,\dots) & \text{degrees of freedom of } i^{\text{th}} \text{ particle} \\ |x_i\rangle & \text{single particle state with eigenvalues } x_i \\ |\psi\rangle & N\text{-particle state} \end{cases}$$

Definition: The permutation operator P_{ij} acts by exchanging particles i and j:

$$P_{ij}\psi(x_1,\dots,x_i,\dots,x_j,\dots,x_N) = \psi(x_1,\dots,x_j,\dots,x_i,\dots,x_N)$$

This generalizes to arbitrary permutations $P \in S_N$ from the symmetric group S_N:

$$\left.\begin{aligned} &P : \{1,\dots,N\} \to \{P(1),\dots,P(N)\} \\ &\Rightarrow P\psi(x_1,\dots,x_N) = \psi(x_{P(1)},\dots,x_{P(N)}) \end{aligned}\right\}$$

Recall that any permutation can be decomposed into transpositions. The permutation is odd (even) if the number of transposition is odd (even).

Properties of P_{ij} and P:

(i) $P_{ij}^2 = \mathbb{1}$

(ii) $\langle \varphi | \psi \rangle = \langle P\varphi | P\psi \rangle$

(iii) $\langle \varphi | P\psi \rangle = \langle P^{-1}\varphi | P^{-1}P\psi \rangle = \langle P^{-1}\varphi | \psi \rangle$

$\Rightarrow \quad P^{+} = P^{-1}, \quad P$ is unitary.

(iv) Because of (i), transposition are also Hermitian.

Indistinguishability implies that for any observable A and any permutation P

$$\begin{cases} \langle \psi | A | \psi \rangle \overset{!}{=} \langle P\psi | A | P\psi \rangle = \\ = \langle \psi | P^{+} A P | \psi \rangle = \\ \Rightarrow \quad A = P^{+}AP \quad \Rightarrow \quad PA = AP \quad \Rightarrow \quad [P, A] = 0. \end{cases}$$

We therefore demand that the basis states of a system of identical particles should be eigenstates of all permutations. In particular, for transposition we demand

$$P_{ij} | \chi \rangle = a_{ij} | \chi \rangle$$

- $P_{ij}^2 = \mathbb{1} \quad \Rightarrow \quad a_{ij} = \pm 1$
- For a given $|\chi\rangle$, either all $a_{ij} = 1$ or -1.

Proof: Any transposition P_{ij} can be decomposed according to

$$\left.\begin{array}{l} P_{ij} = P_{1j}\, P_{2i}\, P_{12}\, P_{2i}\, P_{1j} \\ \Rightarrow \quad \underline{a_{ij}} = a_{1j}^2\, a_{2i}^2\, a_{12} = \underline{a_{12}} \end{array}\right\}$$

States with $a_{ij} = 1$ are called symmetric,
states with $a_{ij} = -1$ are called antisymmetric.

Problem: Because transposition do not generally commute for $N \geq 3$, symmetric or antisymmetric basis state do not span the entire N-particle Hilbert space

$$\mathcal{H}_N = \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \ldots \otimes \mathcal{H}}_{N \text{ factors}}$$

The general structure for $N \geq 3$ is

$$\mathcal{H}_N = \underbrace{\mathcal{H}_N^{(S)} \oplus \mathcal{H}_N^{(A)}}_{\substack{\text{subspaces corresponding}\\ \text{to one-dim. representations of } S_N}} \oplus \underbrace{\mathcal{H}_N^{(1)} \oplus \mathcal{H}_N^{(2)} \oplus \ldots}_{\substack{\text{subspaces corresponding}\\ \text{to higher dimensional}\\ \text{representations of } S_N}}$$

symmetric ($\mathcal{H}_N^{(S)}$), antisymmetric ($\mathcal{H}_N^{(A)}$)

Exercise: $N=3$

Higher-dimensional representations must be excluded, because they would imply that physically indistinguishable states are described by different rays in the Hilbert space.

We therefore require the

Symmetry postulate:

(i) The pure state of a system of identical particles is either symmetric or antisymmetric.

(ii) The Hilbert space of a given system contains only symmetric or only anti-symmetric states.

Particles forming symmetric states are called bosons, particles forming antisymmetric states are called fermions.

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b) Symmetrized and antisymmetrized states

We need to construct suitable basis states for $\mathcal{H}_N^{(S)}$ and $\mathcal{H}_N^{(A)}$. Consider a basis

$$|i\rangle = |1\rangle, |2\rangle, |3\rangle$$

of single particle states, then the natural basis of $\mathcal{H}_N$ is

$$|i_1 .. i_N\rangle = |i_1\rangle_1 \, |i_2\rangle_2 \, .. \, |i_N\rangle_N$$

which expresses that particle α is in state $|i_\alpha\rangle$.

Definition: The symmetrized and antisymmetrized basis states are obtained from

$$S_\pm |i_1 \ldots i_N\rangle := \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (\pm 1)^P P |i_1, \ldots, i_N\rangle$$

where

$$(-1)^P = \begin{cases} 1 & P \text{ even} \\ -1 & P \text{ odd} \end{cases}$$

Properties:

(i) $S_+ |i_1 \ldots, i_N\rangle$ is symmetric, $S_- |i_1 \ldots, i_N\rangle$ is antisymmetric.

Proof: $P_{ij} S_+ |i_1 \ldots, i_N\rangle =$

$$= \frac{1}{\sqrt{N!}} \sum_P \underbrace{P_{ij} P}_{=: P'} |i_1 \ldots, i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{P'} P' |i_1 \ldots, i_N\rangle$$

$$= S_+ |i_1 \ldots i_N\rangle$$

$$P_{ij} S_- |i_1 \ldots, i_N\rangle = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \underbrace{P_{ij} P}_{\substack{P' \text{: odd (even) if} \\ P \text{ is even (odd)}}} |i_1 \ldots, i_N\rangle =$$

$$= -\frac{1}{\sqrt{N!}} \sum_{P'} (-1)^{P'} |i_1 \ldots, i_N\rangle = - S_- |i_1 \ldots, i_N\rangle$$

(ii) <u>If $|i_\alpha\rangle = |i_\beta\rangle$ for some $\alpha \neq \beta$,</u>

<u>then $S_- |i_1 \dots, i_N\rangle = 0$</u> (Pauli principle)

<u>Proof:</u> $S_- |i_1 \dots, i_N\rangle = \frac{1}{\sqrt{N!}} \sum_P (-1)^P P |i_1 \dots, i_N\rangle$

$$= \frac{1}{\sqrt{N!}} \sum_P (-1)^P P P_{\alpha\beta} |i_1 \dots, i_N\rangle = - S_- |i_1 \dots, i_N\rangle$$

$$\Rightarrow \quad S_- |i_1 \dots, i_N\rangle = 0$$

(iii) <u>Normalization of $S_+ |i_1 \dots, i_N\rangle$</u>

If several bosons are in the same single particle state, then $S_+ |i_1 \dots, i_N\rangle$ is not properly normalized. Suppose there are n_k particles in state k, with $k = 1, \dots, M \leq N$. Then $S_+ |i_1 \dots, i_N\rangle$ contains

$$\binom{N}{n_1, n_2, n_3, \dots, n_M} = \frac{N!}{\prod_{k=1}^{M} n_k!}$$

multinomial coefficient

distinct terms, each with a multiplicity of $\prod_k n_k!$. Thus we can write

$$S_+ |i_1 \dots, i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{j=1}^{\binom{N}{n_1 \dots n_M}} \left(\prod_k n_k!\right) |\alpha_j\rangle$$

where the $|\alpha_j\rangle$ are orthonormal. Thus

$$\langle i_1 \ldots, i_N | S_+^\dagger S_+ | i_1 \ldots, i_N \rangle = \frac{1}{N!} \frac{N!}{\prod_k n_k!} \left(\prod_k n_k!\right)^2$$

$$= \prod_{k=1}^{M} n_k!$$

$$\Rightarrow \quad |n_1 \ldots, n_M\rangle = \frac{1}{\sqrt{\prod n_k!}} S_+ |i_1 \ldots, i_N)$$

is a normalized, symmetric basis state

(iv) The $S_\pm |i_1 \ldots, i_N\rangle$ form a complete basis of $\mathcal{H}_N^{(S)}$ and $\mathcal{H}_N^{(A)}$, respectively.

Proof: $|\psi\rangle \in \mathcal{H}_N^{(S)} \Rightarrow P|\psi\rangle = |\psi\rangle \;\forall P$

$$\Rightarrow \frac{1}{\sqrt{N!}} S_+ |\psi\rangle = \frac{1}{N!} \sum_P P|\psi\rangle = |\psi\rangle$$

Hence if $|\psi\rangle = \sum_{i_1 \ldots i_N} c_{i_1 \ldots i_N} |i_1 \ldots i_N\rangle$

then

$$|\psi\rangle = \frac{1}{\sqrt{N!}} S_+ |\psi\rangle = \sum_{i_1 \ldots, i_N} c_{i_1 \ldots, i_N} \frac{1}{\sqrt{N!}} S_+ |i_1 \ldots, i_N\rangle$$

is a representation of $|\psi\rangle$ in terms of the basis $S_+ |i_1 \ldots, i_N\rangle$.

The proof for the antisymmetric case is analogous.

2° Fock space

a) Fock space for bosons

We have seen that the symmetrized N-particle states

$$|n_1 \ldots n_m\rangle = \frac{1}{\left(N! \prod_{k=1}^{m} n_k!\right)^{1/2}} \sum_{P \in S_N} P|i_1, \ldots, i_N\rangle$$

are fully characterized by the occupation numbers n_k of the single particle states:

n_k = number of particles in state $|k\rangle$

with $n_k \geq 0$ and $N = \sum_k n_k$. These states are normalized and orthogonal:

$$\langle n_1 n_2 \ldots | n_1' n_2' \ldots \rangle = \delta_{n_1 n_1'} \delta_{n_2 n_2'} \ldots$$

because of the orthogonality of the single particle states.

We now combine the bosonic N-particle Hilbert spaces $\mathcal{H}_N^{(S)}$ into the Fock space

$$\mathcal{H}_{Fock}^{(S)} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N^{(S)}$$

which is the direct sum of the $\mathcal{H}_N^{(S)}$.

- Elements of $\mathcal{H}^{(S)}_{\text{Fock}}$ are elements of the $\mathcal{H}^{(S)}_{N}$ and their superpositions.
- $\mathcal{H}^{(S)}_{0}$ is the one-dimensional subspace spanned by the vacuum state (no particle)
- $\mathcal{H}^{(S)}_{1} = \mathcal{H}$ is the single particle Hilbert space spanned by the states

  $|n_1=0, n_2=0, .., n_k=1, n_{k+1}=0, .., \rangle = |k\rangle$
- The basis states of $\mathcal{H}^{(S)}_{\text{Fock}}$ are the union of the basis states of the $\mathcal{H}^{(S)}_{N}$,

  $|n_1, n_2, n_3 .. \rangle$ with $n_k \geq 0$ and no constraint on $\sum n_k$.
- In particular, the completeness relation

$$\sum_{n_1, n_2, ..} |n_1\, n_2\, ..\rangle\langle n_1\, n_2\, ..| = \mathbb{1}$$

  holds.

Standard N-particle operators only act within the N-particle sector of $\mathcal{H}^{(S)}_{\text{Fock}}$. To connect different sectors we introduce annihilation and creation operators:

Define first the creation operator:

$$a_i^\dagger \underbrace{|n_1 \ldots, n_i \ldots\rangle}_{\text{in } \mathcal{H}_N^{(S)}} = f(n_i) \underbrace{|n_1 \ldots n_i+1 \ldots\rangle}_{\text{in } \mathcal{H}_{N+1}^{(S)}}$$

$$\Rightarrow \langle n_1', \ldots, n_i' \ldots | a_i = f(n_i')^* \langle n_1' \ldots n_i'+1 |$$

$$\Rightarrow \langle n_1' \ldots n_i' \ldots | a_i | n_1 \ldots n_i \ldots \rangle =$$

$$= f^*(n_i') \, \delta_{n_1 n_1'} \ldots \underbrace{\delta_{n_i'+1, n_i}}_{=1 \text{ if } n_i' = n_i - 1}$$

$$\Rightarrow a_i |n_1 \ldots n_i \ldots\rangle = \begin{cases} 0 & n_i = 0 \\ f^*(n_i - 1) \, |n_1 \ldots n_i - 1, \ldots\rangle & \text{if } n_i > 0 \end{cases}$$

$\Rightarrow$ a_i is an annihilation operator.

To fix the function $f(n)$ we consider the operator

$$N_i = a_i^\dagger a_i$$

For $n_i > 0$ we have

$$N_i | \ldots n_i \ldots \rangle = a_i^\dagger f^*(n_i - 1) | \ldots n_i - 1 \ldots \rangle$$

$$= |f(n_i - 1)|^2 | \ldots n_i \ldots \rangle$$

$\Rightarrow$ $| \ldots n_i \ldots \rangle$ is an eigenstate of N_i

with eigenvalue $|f(n_i - 1)|^2$. With the choice

$$\underline{f(n_i) = \sqrt{n_i + 1}}$$

the eigenvalue is the number of particles in state i

$$\Rightarrow \begin{cases} N_i = a_i^\dagger a_i & \text{particle number operator in state } i \\ \hat{N} = \sum_i N_i & \text{total particle number operator} \end{cases}$$

To summarize:

$$a_i^\dagger | \ldots n_i \ldots \rangle = \sqrt{n_i + 1} \, | \ldots n_i + 1 \ldots \rangle$$

$$a_i | \ldots n_i \ldots \rangle = \begin{cases} 0 & n_i = 0 \\ \sqrt{n_i} \, | \ldots n_i - 1 \ldots \rangle & \text{else} \end{cases}$$

This implies in particular

$$\left. \begin{aligned} a_i^\dagger a_i | \ldots n_i \ldots \rangle &= n_i | \ldots n_i \ldots \rangle \\ a_i a_i^\dagger | \ldots n_i \ldots \rangle &= (n_i + 1) | \ldots n_i \ldots \rangle \end{aligned} \right\}$$

$$\Rightarrow \underline{[a_i, a_i^\dagger] = 1}$$